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Modeling of low-speed rarefied gas flows using a combined ES-BGK/DSMC approach

(Preprint)

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Modeling of low speed gas flows at moderate Knudsen numbers, where conventional continuum CFD methods are inapplicable and kinetic methods are either inaccurate of prohibitively expensive, presents a significant challenge for computational modeling. In this work, an approach that combines a finite-volume solution of the ES-BGK model kinetic equation and the statistical DSMC method to accurately predict radiometric forces on a vane in large vacuum chamber filled with rarefied gas is presented. The approach in effect combines the accuracy of a statistical solution of the Boltzmann equation with the numerical efficiency of a deterministic solution of simplified model kinetic equations.

Keywords: DSMC, ES-BGK, radiometric, low-speed flow

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I. Introduction

The repulsion and attraction of bodies induced by radiation was drawing attention of a number of prominent scientists in the 19th and 20th centuries.[1] The first published experiment was conducted by Abraham Bennet,[2] who in 1792 reported that when the light was shined on a paper vane suspended on a fiber thread in a vacuum, there was no motion distinguishable from the effect of heat. The first successful experiment was conducted by Fresnel[3] who in 1825 observed a repulsion between two foil vanes suspended in a low-pressure container when sunlight was focused on them. In 1870s, William Crookes proposed different types of apparatus to investigate the radiometer effect;[4] one of them has later become known as Crookes radiometer. Crookes incorrectly suggested that the force was due to the pressure of light.

The first correct explanation of the radiometric phenomena was presented by Reynolds,[5] who used the main principles of the kinetic theory of gases for his explanation. The molecules with higher velocities that leave the hot side of the vane collide with the oncoming molecules, and cut the surface momentum flux more efficiently than those reflected from the cold surface. At about same time, Maxwell[6] has also showed that an unbalanced force exists near the edge of the heated side of the vane, where the heat flow in the gas in non-uniform. Almost fifty years later, Einstein presented a simple theory[7] that related the force on the vanes to their perimeter. This edge dependence of the vane force has found partial confirmation in experimental work,[Marsh (1926)] where the force was found to depend on perimeter, although the dependence was weaker than the linear dependence predicted by Einstein.

Significant interest drawn by the radiometer problem between 1870 and 1930 had been declining after that, both because the issue was considered closed, and because no direct application for radiometric forces has been found at that time. The situation started to change in 1990s, when the radiometric phenomena was found useful in a number of different micro- and large scale devices. One of the most important of these is atomic force microscopy, a research field that, although invented back in 1980s,[8] has been brought to the forefront of modern nanotechnologies in the last several years (see, for example,[9]). The radiometric force has also been shown to be applicable to modern microactuators in,[10] where the direct simulation Monte Carlo (DSMC) method has been used to model forces on vanes mounted on an armature. This method, along with experimental measurements, have been employed in[11] to study a concept of an opto-microengine that uses radiometric forces. Then, the work of Passian with co-workers have been published

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(see, for example,,[12] where radiometric phenomena were studied experimentally and analytically, mostly in application to microcantilevers). Radiometric force as an approach to study gas-surface translational energy accommodation has been mentioned by Passian et al in.[13] A new concept of a high-altitude aircraft supported by microwave that uses radiometric effects has been put forward in.[14] Most recently, the contribution of the edge and the area forces to the total radiometric force was examined experimentally and numerically in,[15] the mechanism of the edge force formation was studied in,[16] and a new method for obtaining gas-surface accommodation coefficients was proposed in.[17] The method utilizes the fact that radiometric forces exerted on heated objects immersed in rarefied gases are governed by the interaction of gas molecules with the surface, and is based on the matching of measured and computed radiometric forces.

A number of numerical and physical problems associated with radiometric flows make accurate calculation of forces on radiometer vanes extremely, and often prohibitively, expensive, even for modern parallel computers. The problems arise mostly because the conventional techniques, such as those based on the solution of the Navier-Stokes equations, are inapplicable, since the near-equlibrium assumptions on stress and heat flux are not valid for significantly non-equilirbiom, rarefied radiometric flows. A kinetic, microsopic approach has therefore to be used to properly account for temperature gradients and shear streasses inherent in radiometric flows. Kinetic methods, which explicitely calculate the molecular velocity distribution functions, while usually are more robust and accurate than the continuum methods, lack the numerical efficiency of the latter.

The main objective of the present work is to bridge two kinetic methods, the numerical solution of model kinetic equations and the DSMC method. The model kinetic equations are simplifications of the Boltzmann equation, which is the governing equation of the non-equilirbium gas dynamics. For low speed flows, the DSMC method, which represents a statistical solution to the Boltzmann equation, is much more expensive, but at the same time more accurate than any solution of a model kinetic equation. The proposed approach is effectively an overlay approach, where a model kinetic equation is solved in the entire field of interest, and then the DSMC method is applied only in a small area of most importance, which in the radiometer case is the region adjacent to the vane.

II. Challenges of numerical modeling of low speed flows

There are several challenges in the radiometric flow modeling, most of which are related to the low speed nature of these flows. The principal challenges are modeling of subsonic boundary conditions, low signal-to-noise ratio, and very long time to reach steady state. The first problem may be overcome when a closed system is considered; in this case, the wall boundary conditions may be imposed on the boundaries of the computational domain. However, the study of the accommodation coefficients implies that a very large chamber needs to be considered to avoid the impact of the chamber walls. The physical problem of the boundary conditions is therefore replaced by a computational problem of a large simulation domain. The low signal-to-noise ratio is mostly a challenge for statistical kinetic approaches, such as the direct simulation Monte Carlo (DSMC) method.[18] Very long times to reach steady state create difficulties primarily for time-accurate approaches where the use of an implicit method may solve these problems.

There are a number of kinetic approaches that are generally capable of predicting radiometric flows; they all differ in the degree of precision and the computational cost. At present, the most powerful and widely used kinetic approach to the solution of the Boltzmann equation is the DSMC method. This approach however suffers from high computational cost when low-speed flows need to be modeled. There is a number of alternative DSMC-based approaches proposed to deal with the problem of low signal-to-noise ratio that allow significant reduction in macroparameter sampling time compared to the standard DSMC method (see, for example,[19,20]). Although all these techniques do allow significant reduction in the steady-state time averaging cost, they do not deal with the reduction of computational cost associated with the long time to reach steady state, which is often the main issue for modeling radiometric flows. The direct numerical integration of the Boltzmann equation,[21] while avoiding the signal-to-noise ratio problem, may be impractical when millions of time steps and tens or hundreds of thousands of cells have to be modeled.

A plausible numerical alternative for such flows appears to be a deterministic solution of a simplified form of the Boltzmann equation known as a kinetic model equations. Bhatnagar-Gross-Krook (BGK)[22] and ellipsoidal statistical (ES)[23] kinetic models use a non-linear relaxation term instead of the full Boltzmann collision integral, and possess the same collision invariants as the Boltzmann equation. Both BGK and ES models satisfy the H-theorem[24] expressing the increase of entropy of gas under consideration. The ES model seems preferable as it allows one to use the correct Prandtl number, whereas the Prandtl number

for the BGK model is unity. The primary advantage of this numerical alternative is its high computational efficiency.

III. Modeling of radiometric flows with DSMC and ES-BGK methods

Numerical analysis has been conducted using the DSMC and ES-BGK methods in order to assess their applicability to modeling of radiometric flows in general, and the experimental setup described in the previous section, in particular. The computational tool SMILE[25] was used to obtain the solutions with the DSMC method. In DSMC runs, the variable soft sphere model (VSS) with parameters listed in Ref.[18] was used for the molecular collisions, and the Maxwell model was used to calculate gas-surface collisions. A finite volume solver SMOKE[26] has been used to deterministically solve the ES model kinetic equation. SMOKE is a parallel code based on conservative numerical schemes developed in.[27] A second order spatial discretization was used. The solutions were typically obtained in two successive steps. First, an implicit time integration scheme was run until the result is converged. Second, a conservative explicit time integration scheme was used with the initial conditions from the first step. This two-step approach allowed up to two orders of magnitude reduction in computational time compared to an explicit-only case.

The computations presented in this section were conducted for a two-dimensional chamber of 0.44m×0.44m. The size of the vane was 0.04m×0.01m. The vane temperatures were 450 K and 410 K for the hot and cold sides, respectively. A chamber wall temperature of 300 K was assumed. The computations were performed for pure argon. The results for a stagnation pressure of 0.609 Pa are presented in Fig. 1, where the translational temperature fields are presented for the ES-BGK (upper half) and DSMC (lower half) solutions. As expected, the gas temperature significantly increases near the vane. For this pressure, which corresponds to the Knudsen number of approximately 0.25 based on the vane height, the temperature jump at the surface is about 40 K for the hot side, and 30 K for the cold side. At the chamber walls, the temperature jump is about 2 K. The main conclusion from the comparison of the two solutions is that they agree very well, both in the regions close to the vane and near the chamber walls. The difference between the solutions is less than one degree Kelvin, which is reasonably small compared to the temperature variation from chamber walls to the radiometer vane, which exceeds 100 K.

Comparison of the argon number density fields for the two approaches is given in Fig. 2. There is

generally very good quantitative agreement between the DSMC and ES-BGK solutions. The difference does not exceed a few tenths of a percent, which is within the numerical error of the calculations, estimated to be below 1%, and mostly related to the spatial and time discretization, as well as the number of molecules in the DSMC method.

Good agreement between the macroparameters obtained with the statistical and deterministic kinetic approaches allows one to assume equally good agreement between the surface properties. The pressure forces calculated are indeed close both for the hot and the cold sides of the plate. For the DSMC calculation, the integral pressure force is 2.4928×10^{-2} N and 2.4627×10^{-2} N for the hot and the cold sides, respectively. For the ES-BGK calculation, these values are 2.4926×10^{-2} N and 2.4664×10^{-2} N. However, the radiometric force is based on the difference between the hot and the cold side forces, giving 3.01×10^{-4} N in DSMC and 2.62×10^{-4} N in ES-BGK. Therefore, the difference in the radiometric forces between the two numerical techniques is almost 15%. The radiometric force only amounts to about one percent of the pressure force on the hot surface, and its accurate calculation is difficult.

The results for the radiometric pressure-based force on the vane are given in Fig. 3. These results show that the DSMC and ES-BGK forces coincide in the free molecular regime, as expected, and are close for larger pressures (for Knudsen numbers smaller than 0.1). However, for intermediate pressures the DSMC values are systematically higher, with the maximum difference observed at 0.609 Pa. This deviation of the BGK solution from DSMC is attributed to the approximations inherent in the ES-BGK model equation as compared to the full Boltzmann equation that is solved statistically with the DSMC method. The collision operator of the model kinetic equation is such that the relaxation of molecules that have different velocities occurs at the same speed; in addition, the relaxation of molecules after collisions to the local Maxwellian distribution is not a satisfactory assumption under strongly non-equilibrium conditions.

IV. Combined ES-BGK/DSMC approach

Accurate modeling of flow macroparameters and significant underprediction of the radiometric force by the solution of the ES-BGK equation indicates that the approach may be used for a qualitative analysis of radiometric phenomena, but not for the quantitative prediction of radiometric forces. On the other hand, the use of the DSMC method to compute radiometric forces in large chambers, necessary to avoid chamber

wall effects, is prohibitively computationally expensive. A reasonable alternative appears to be the use of a combined ES-BGK/DSMC approach, where the final solution is obtained in two successive steps. First, an ES-BGK modeling is conducted in a large computational domain that includes both the radiometer vane and the chamber walls. The solution of this first step is used to set the boundary conditions for the second step. At the second step, the DSMC method is applied in a much smaller domain, with the subsonic boundary conditions taken from the first step.

There are a number of ways to specify the boundary conditions for DSMC. The easiest one is to directly use the four macroparameters (density, temperature, and two velocities) from the ES-BGK solution in the DSMC simulations. In this case, the velocities of molecules entering the DSMC computational domain are sampled from the Maxwellian distribution with parameters from the ES-BGK solution. Another possibility is to use directional temperatures obtained from the ES-BGK solution, and sample velocities of new molecules in DSMC from the ellipsoidal distribution function. Finally, the most accurate, and the most cumbersome, way to set the DSMC boundary conditions is to use the velocity distribution functions from the solution of the model kinetic equation.

One way to examine the applicability of various approaches to the boundary conditions is to apply a combined ES-BGK/DSMC method to a test case where a reliable DSMC solution is available for the entire chamber, and then compare the obtained results. In this work, the DSMC solution presented earlier was chosen as the validation tool for the combined approach. The computational domain for the DSMC step of the combined approach was set to 0.22m×0.22m (one half of the full chamber size in each direction). The range of pressures from 0.3 Pa to 3 Pa was considered in order to examine the flow regime where the difference in radiometric force between the DSMC and ES-BGK methods is most pronounced. For the case under consideration, analysis of nonequilibrium between the directional temperatures showed that the difference between T_x and T_y along the boundaries of the DSMC domain in the combined approach does not exceed 0.2%, and typically is less than 0.1%. Because of this, the approaches based on Maxwellian and ellipsoidal distributions of incoming molecules are expected to produce results that agree within the numerical error of the computations. Therefore, only the Maxwellian distribution was used below.

It is much more important to separate the incoming and outgoing fluxes of molecules in the ES-BGK solution when setting up the boundary conditions for the second-step DSMC simulation. The gas temperature

of the incoming molecules is significantly (several percent) smaller than that based on both incoming and outgoing molecules. The resulting pressure force for the combined ES-BGK/DSMC approach that uses either total incoming and outgoing molecules or the incoming molecules alone is given in Table 1. The corresponding DSMC values are also shown in this table. The incoming molecule based ES-BGK/DSMC force practically coincides with the benchmark DSMC values for lower and higher pressures. It is slightly larger than the DSMC near the maximum. The force obtained using the total properties is larger for all pressures under consideration; the difference is especially significant for higher pressures.

The combined ES-BGK/DSMC approach, while providing results close to those of the DSMC method, allows for significant reduction in the computational time as compared to the DSMC method. In the example considered above, the DSMC modeling took from 1,500 CPH for lower pressures to 3,000 CPH for higher pressures cases. The combined approach allowed to reduce these numbers by approximately a factor of three. Even though it is longer than it takes to solve the ES-BGK equation (about 10 to 30 CPH depending on gas pressure), it is at the same time much closer to the DSMC solutions than ES-BGK.

Good agreement between the incoming properties based ES-BGK/DSMC approach and the DSMC-only solution proves that the combined method may be used for the evaluation of radiometric forces in situations where the application of the DSMC method is ether impracticale or impossible. One example given here is the computation of the radiometric forces on a circular 5.5 cm vane immersed in a very large, 3 m diameter vacuum chamber. The force on such a radiometer was measured in.[17] Note that since the radiometic force was found to be very sensitive to the size of the computational domain,[15] the actual 3 m sized vacuum chamber used in the experiments has to be simulated numerically. Modeling of a low-speed, slowly converging flow with a Knudsen number on the order of 0.001, based on the chamber diameter, using the DSMC method would require the run time of millions CPH, making such runs virtually impossible. The long run time is due to slow convergence, low signal-to-noise ratio, and the fact that the radiometric force is the difference between the forces on the hot and cold sides of the vane, and typically is less than one percent of the force on either cold or hot side.

The combined ES-BGK/DSMC approach makes such a large-chamber modeling possible. Comparison of the present numerical and experimental[17] results on the radiometric force in pure argon is shown in Table 2. To reproduce experimental conditions of,[17] an axisymmetric 3m×1.5 m computational domain

bounded by the chamber walls was used in the ES-BGK computations. A much smaller axisymmetric 0.3m$\times$0.3m computational domain was taken in the DSMC modeling. The total run time was on the order of 5,000 CPH. Note that the Maxwell model with an incomplete accommodation of 0.8 was used for the gas-surface interactions, which is a reasonable value for an argon-aluminum interaction.[17, 28] Generally, there is an acceptable agreement between the ES-BGK/DSMC and experimental results. At the same time, the ES-BGK force is close to the experimental value only in the nearly free-molecular regime, while significantly underpredicting the data in the transitional regime.

V. Conclusions

An approach that combines the deterministic solution of the ES-BGK model kinetic equation and the DSMC method in an overlay mode to compute low speed radiometric type flows is presented. In this approach, the final solution is obtained in two steps. First, an ES-BGK modeling is conducted in a large computational domain that includes both the radiometer vane and the chamber walls. The solution of this first step is used to set the boundary conditions for the second step. At the second step, the DSMC method is applied in a much smaller domain, with the subsonic boundary conditions taken from the first step. The macroparameters for these subsonic boundary conditions are based only on the incoming fluxes. The use of such an approach is recommended based on the fact that DSMC modeling of a radiometric flow on a 10 cm vane in a 3 m chamber, where the accuracy of the radiometric force modeling needs to be on the order of 1%, is prohibitively expensive, whereas the ES-BGK method, while being accurate enough in terms of gas flowfields, produces an error up to 15% in the radiometeric force. The combined ES-BGK method was found to agree well both in the DSMC results in a small chamber, and experimental data in a large chamber.

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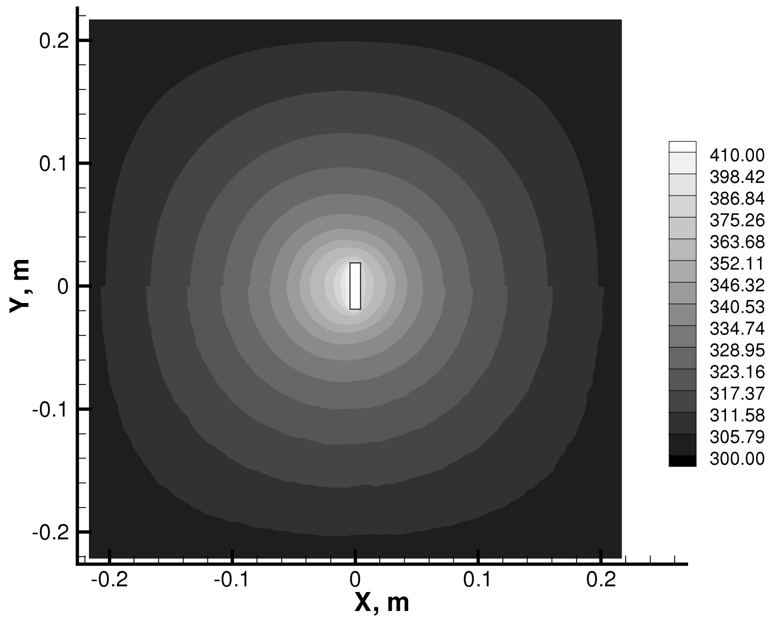

Figure 1. ES-BGK (top) and DSMC (bottom) translational temperature fields.

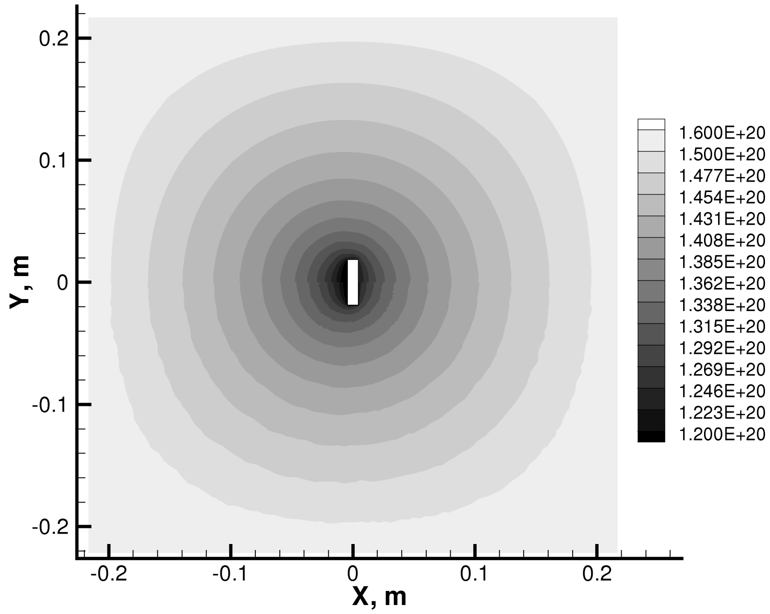

Figure 2. ES-BGK (top) and DSMC (bottom) number density fields.

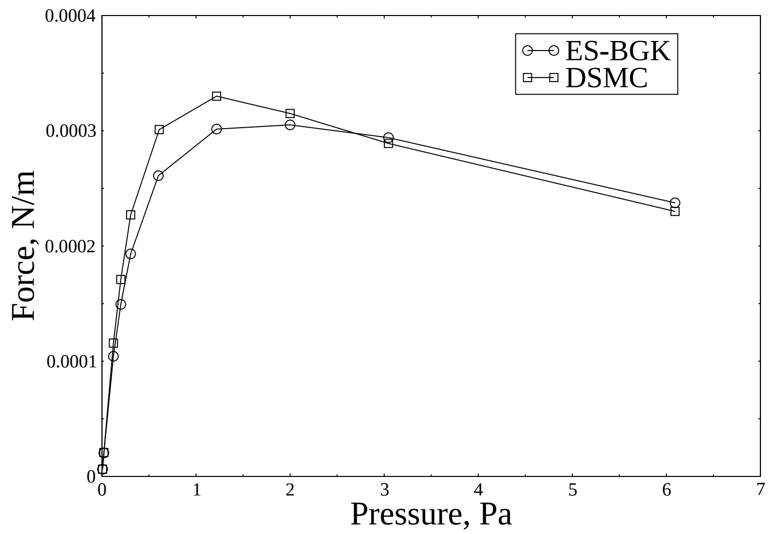

Figure 3. Radiometric forces on the plate obtained with ES-BGK and DSMC.

Pressure, Pa	DSMC	ES-BGK	ES-BGK/DSMC incoming	ES-BGK/DSMC total
0.305	2.27e-4	2.14e-4	2.28e-4	2.33e-4
0.609	3.01e-4	2.62e-4	3.00e-4	3.07e-4
1.219	3.30e-4	2.97e-4	3.40e-4	3.56e-4
2.000	3.15e-4	2.96e-4	3.26e-4	3.38e-4
3.046	2.89e-4	2.81e-4	2.85e-4	3.32e-4

Table 1. Comparison of radiometric forces (N) obtained with different approaches in a small 2D chamber.

Pressure, Pa	ES-BGK	ES-BGK/DSMC incoming	Experiment
0.012	1.662e-6	1.594e-6	1.631e-6
0.066	7.551e-6	9.001e-5	8.900e-6
0.299	1.825e-5	2.188e-5	2.245e-5
0.596	2.147e-5	2.587e-5	2.473e-5
0.954	2.162e-5	2.378e-5	2.292e-5

Table 2. Comparison of numerical and experimental radiometric forces (N) in a large axisymmetric chamber.